

Core Community Specifications for Electron Microprobe Operating Systems: Software, Quality Control, and Data Management Issues

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Modern electron microprobe systems have become increasingly sophisticated. These systems utilize either UNIX or PC computer systems for measurement, automation, and data reduction. These systems have undergone major improvements in processing, storage, display, and communications, due to increased capabilities of hardware and software. Instrument specifications are typically utilized at the time of purchase and concentrate on hardware performance. The microanalysis community includes analysts, researchers, software developers, and manufacturers, who could benefit from exchange of ideas and the ultimate development of core community specifications (CCS) for hardware and software components of microprobe instrumentation and operating systems.

Is this needed? We think it is. Analysts are required, under ISO 9000, to maintain documentation records demonstrating the steps taken in calibrating their equipment and procedures (i.e., standards, blanks, detection limits, analytical error, periods between recalibration, etc). These records are either formally required via ISO structure, or implicitly necessary as many experienced probe users have expressed the desire for improved handling and storage of data, to ensure that critical parameters are saved automatically (e.g., not having to write down in a notebook the date the most recent peaking was done) and that essential basic standardization or measurement information is not deleted or overwritten.

Microprobe facilities must be able to document quality control (QC) and data integrity as part of ISO 9000 programs. Ongoing efforts of ISO9000/TC 202 serve to establish documentation for hardware components of microanalysis systems, but software issues have yet to be discussed in detail. The analysis of mission critical materials as part of coordinated testing and analysis programs places increased demands on the analyst to provide quality assurance information and to verify the internal consistency of data sets acquired at different times in the analysis program. At a fundamental level this requires data linking and database management tools that include time stamps on all activities. The following examples are a summary of discussions among a small group of analysts based on their needs.

Specifically, the periodic demonstration of alignment of the wavelength-dispersive spectrometers (WDS), characterization of detector dead-time, and pulse-height analysis (PHA) and counting system, must be conveniently performed and readily available. All EDS, WDS, imaging, measurement, composition, and other analytical data should be accessible in a database format that allows for inspection, summary, and manipulation, and which allows tools that can be modified by users for extraction of data. The primary standardization data should include the identity and composition of the standard, spectrometer peaking information and record of the peak profile data, individual count data from each background and peak intensity at each sampled point, and the ability to inspect and select count data at a time after the run was conducted. The standard intensity and composition data should be compared to other data from other runs in order to evaluate long-term stability and accuracy. Sample data should include a complete record of the probe current and absorbed current stability during the

measurement, and an EDS spectrum should be archived for all analyses in order to document the composition and possible charging characteristics of the sample in a post-run review. Most operating systems do not provide adequate information regarding propagated analytical uncertainty and detailed statistical information for use on sets of measurements. The ability to acquire WDS k-ratio data in digital compositional maps, corrected using full $\phi(\rho z)$ quantitative correction, has yet to be implemented. The powerful capabilities of spectrum imaging software and data cube management should be added to basic microprobe operating system capabilities.

The EMSA EDS format for EDS data files was an important step for platform independent access to EDS spectral data. More recent work has included development of an xml format. An equivalent independent file format is needed for microprobe data that includes EDS and WDS spectrum data, quantitative analysis data, image files, data cubes, and other types of data produced on modern instruments. Several issues exist with current operating systems, as analytical data is neither co-located nor linked to other data acquired during a given session. Provisions for multi-user accounts on microprobes have not adequately protected primary standardization data from use, modification, or deletion by other users.

There currently is no standard template for specifying which EPMA parameters are to be preserved in an analytical session. We suspect that much of today's probe software's structure is a direct descendant of the days when 64K was a large amount of memory, hard disks were a luxury and 8 inch floppies were the storage mode. Given the luxuries we have with microprocessors, memory and hard disk space, today's instruments should provide increased flexibility to users in storing data for later retrieval and post processing. It should be possible, for example, to provide quality assurance data during an analytical run by automated bracketing of unknowns with standards, as well as the ability to correct for a limited range of errors after a run has been completed. For example, background correction in WDS measurement involves selection of background offsets during initial setup, and should include an assessment of background intensity during sample measurement. This monitoring, coupled with a sophisticated peak interference correction capability, helps avoid analytical errors during a run, and allows recovery both during and after the run via post-processing.

Current microprobe systems utilize and produce large volumes of data with selective storage of data as determined necessary by the software developers. It can be scattered across the hard disk in many different locations (calibration positions in one file, calibration counts in another, wavelength scans in another, images in another, etc). It seems that a database organization of data storage, with flexible selection of storage parameters by the analyst, offers much in the way of future capability, and reduces vulnerability to issues where data is not co-located.

We introduce this line of discussion and invite input from analysts, researchers, software developers, and manufacturers. As we leave 50 years of historical development of EPMA on the history books, we seek to bring new capabilities in terms of hardware and software to the technique.